

# GROUND STATE ENERGY OF LARGE POLARON SYSTEMS

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**ABSTRACT.** The last unsolved problem about the many-polaron system, in the Pekar–Tomasevich approximation, is the case of bosons with the electron-electron Coulomb repulsion of strength exactly 1 (the ‘neutral case’). We prove that the ground state energy, for large  $N$ , goes exactly as  $-N^{7/5}$ , and we give upper and lower bounds on the asymptotic coefficient that agree to within a factor of  $2^{2/5}$ .

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## 1. INTRODUCTION AND MAIN RESULTS

In this paper we are concerned with the ground state energy of a system of  $N$  polarons in the Pekar–Tomasevich approximation [PT], which is derived from the Fröhlich polaron [F], in the limit of large coupling constant  $\alpha$  (see (1.7)). The Pekar–Tomasevich energy functional is

$$\mathcal{E}_U^{(N)}[\psi] = \int_{\mathbb{R}^{3N}} \left( \sum_{j=1}^N |\nabla_j \psi|^2 + U \sum_{j < k} \frac{|\psi|^2}{|x_j - x_k|} \right) dx - D(\rho_\psi, \rho_\psi) \quad (1.1)$$

for  $\psi \in H^1(\mathbb{R}^{3N})$  with  $\int_{\mathbb{R}^{3N}} |\psi|^2 dx = 1$ . (We will write  $\|\psi\|$  to denote the  $L^2$ , not the  $H^1$  norm.) We have used the usual notations

$$\rho_\psi(x) = \sum_{j=1}^N \int \cdots \int_{\mathbb{R}^{3(N-1)}} |\psi(x_1, \dots, x_{j-1}, x, x_{j+1}, \dots, x_N)|^2 dx_1 \dots dx_{j-1} dx_{j+1} \dots dx_N$$

for the particle density corresponding to  $\psi$  and

$$D(\rho, \sigma) = \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\overline{\rho(x)} \sigma(x')}{|x - x'|} dx dx'$$

for the Coulomb energy. The dimensionless parameter  $U > 0$  in (1.1) describes the strength of the Coulomb repulsion between the particles relative to the strength of their self-attraction. (Originally, there is another parameter  $\alpha > 0$  in front of  $D(\rho_\psi, \rho_\psi)$ , but by scaling we may assume that  $\alpha = 1$ .)

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We are concerned both with the case of bosonic and of fermionic statistics and we denote the corresponding ground state energies by

$$E_U^{(b)}(N) = \inf \left\{ \mathcal{E}_U^{(N)}[\psi] : \text{symmetric } \psi \in H^1(\mathbb{R}^{3N}), \int_{\mathbb{R}^{3N}} |\psi|^2 dx = 1 \right\}$$

and

$$E_U^{(f)}(N) = \inf \left\{ \mathcal{E}_U^{(N)}[\psi] : \text{antisymmetric } \psi \in H^1(\mathbb{R}^{3N}), \int_{\mathbb{R}^{3N}} |\psi|^2 dx = 1 \right\}.$$

For simplicity, we ignore spin. It is well known that  $E_U^{(b)}(N)$  coincides with the infimum of  $\mathcal{E}_U^{(N)}[\psi]$  over all  $\psi \in H^1(\mathbb{R}^{3N})$  with  $\int_{\mathbb{R}^{3N}} |\psi|^2 dx = 1$ , that is, the assumption ‘symmetric’ in the definition of  $E_U^{(b)}(N)$  can be dropped. This implies, in particular, that  $E_U^{(b)}(N) \leq E_U^{(f)}(N)$  for all  $N \in \mathbb{N}$ .

Let us review what is known about the large  $N$  behavior of  $E_U^{(b)}(N)$  and  $E_U^{(f)}(N)$ . These results depend crucially on the sign of  $U - 1$ . For  $U < 1$  and fermions it is shown in [GM] that

$$-\infty < \liminf_{N \rightarrow \infty} N^{-7/3} E_U^{(f)}(N) \leq \limsup_{N \rightarrow \infty} N^{-7/3} E_U^{(f)}(N) \leq e_U^{(f)}, \quad (1.2)$$

for some explicit constant  $e_U^{(f)}$  (defined in (1.9) below). We shall prove that both  $\leq$  in (1.2) are  $=$ , in fact. For  $U < 1$  and bosons it was noted in [FLST] that  $\liminf_{N \rightarrow \infty} N^{-3} E_U^{(b)}(N)$  and  $\liminf_{N \rightarrow \infty} N^{-3} E_U^{(f)}(N)$  are finite and in [BB] it was shown that

$$\lim_{N \rightarrow \infty} N^{-3} E_U^{(b)}(N) = e_U^{(b)}$$

for some explicit constant  $e_U^{(b)}$ . Note that in these cases the thermodynamic limit does not exist.

The situation changes when  $U > 1$ . In this case it was shown in [FLST] that  $\liminf_{N \rightarrow \infty} N^{-1} E_U^{(f)}(N) \geq \liminf_{N \rightarrow \infty} N^{-1} E_U^{(b)}(N) > -\infty$  and it was deduced that

$$\lim_{N \rightarrow \infty} N^{-1} E_U^{(b)}(N) \quad \text{and} \quad \lim_{N \rightarrow \infty} N^{-1} E_U^{(f)}(N) \quad \text{exist.}$$

In the critical case  $U = 1$ , (also known as the neutral case) for fermions, it is shown in [GM] that  $\liminf_{N \rightarrow \infty} N^{-1} E_U^{(f)}(N) > -\infty$ . By the same sub-additivity argument as in [FLST] this implies that

$$\lim_{N \rightarrow \infty} N^{-1} E_1^{(f)}(N) \quad \text{exists.}$$

Thus, our understanding of polaron ground state energies is complete except for the bosonic case with  $U = 1$ . Our goal in this paper is to fill this gap. The following is our main result.

**Theorem 1.1.** *In the bosonic case with  $U = 1$ ,*

$$-2^{2/5} A \leq \liminf_{N \rightarrow \infty} N^{-7/5} E_1^{(b)}(N) \leq \limsup_{N \rightarrow \infty} N^{-7/5} E_1^{(b)}(N) \leq -A, \quad (1.3)$$

where

$$-A = \inf \left\{ \int_{\mathbb{R}^3} |\nabla \varphi|^2 dx - I_0 \int_{\mathbb{R}^3} |\varphi|^{5/2} dx : \varphi \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} |\varphi|^2 dx = 1 \right\}. \quad (1.4)$$

with

$$I_0 = \frac{2}{5} \left( \frac{2}{\pi} \right)^{1/4} \frac{\Gamma(3/4)}{\Gamma(5/4)} \simeq 0.60868. \quad (1.5)$$

We emphasize that (1.3) identifies the correct growth rate of  $E_1^{(b)}(N)$  as  $N \rightarrow \infty$ . Our asymptotic upper and lower bound, however, differ by a factor of  $2^{2/5}$ . We believe that the upper bound is the correct one. Our proof of the theorem is constructive and leads to explicit error bounds. For instance, for the upper bound, we obtain

$$E_1^{(b)}(N) \leq -AN^{7/5}(1 - CN^{-1/35}). \quad (1.6)$$

*Remark 1.2.* Consider the Fröhlich Hamiltonian [F],

$$H_{U,\alpha}^{(N)} = \sum_{j=1}^N (-\Delta_j + \sqrt{\alpha}\varphi(x_j)) + U \sum_{i<j} |x_i - x_j|^{-1} + \int_{\mathbb{R}^3} a_k^* a_k dk \quad (1.7)$$

in  $L_{\text{symm}}^2(\mathbb{R}^{3N}) \otimes \mathcal{F}(L^2(\mathbb{R}^3))$ , where  $\mathcal{F}$  denotes the bosonic Fock space and where

$$\varphi(x) = \frac{1}{2\pi} \int_{\mathbb{R}^3} (a_k e^{ik \cdot x} + a_k^* e^{-ik \cdot x}) \frac{dk}{|k|},$$

with annihilation and creation operators  $a_k$  and  $a_k^*$ . Since a (rescaled) Pekar functional [P] is an upper bound on  $\inf \text{spec } H_{U,\alpha}^{(N)}$  [FLST], we conclude from Theorem 1.1 that for  $U = \alpha$ ,

$$\limsup_{N \rightarrow \infty} N^{-7/3} \inf \text{spec } H_{\alpha,\alpha}^{(N)} \leq -A\alpha^2.$$

In particular, the thermodynamic limit does not exist. If the particles are treated as fermions, the existence of such a limit is still an open problem. *End of Remark*

In our second theorem, proved in the appendix, we show that the upper bound obtained in [GM] in the fermionic case for  $U < 1$  is, in fact, asymptotically correct.

**Theorem 1.3.** *In the fermionic case with  $0 < U < 1$ ,*

$$\lim_{N \rightarrow \infty} N^{-7/3} E_U^{(f)}(N) = e_U^{(f)}, \quad (1.8)$$

with

$$e_U^{(f)} = \inf \left\{ \frac{3}{5} (6\pi^2)^{2/3} \int_{\mathbb{R}^3} \rho^{5/3} dx - (1 - U) D(\rho, \rho) : \rho \geq 0, \int_{\mathbb{R}^3} \rho dx = 1 \right\}. \quad (1.9)$$

We emphasize that the proof of Theorem 1.1 is much more involved than that of Theorem 1.3, which we include mostly for the sake of completeness.

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## 2. PROOF OF THEOREM 1.1

**2.1. The lower bound.** Oddly enough, the *lower* bound is the easy one for us because we have available the results in [LS2] for the two-component charged Bose gas. With its use we can deduce our lower bound from an asymptotic lower bound for the two-component charged Bose gas. Let us recall this result. Given a vector  $e = (e_1, \dots, e_N) \in \{-1, 1\}^N$  (representing charges) we introduce the Hamiltonian

$$H^{(N)}(e) = \sum_{j=1}^N (-\Delta_j) + \sum_{i < j} \frac{e_i e_j}{|x_i - x_j|} \quad \text{in } L^2(\mathbb{R}^{3N}).$$

In [LS2] it is proved that

$$\inf_{e \in \{-1, 1\}^N} \inf \text{spec } H^{(N)}(e) \geq -AN^{7/5} (1 + o(1)), \quad (2.1)$$

where  $A$  is as in (1.4). (Note that we rescaled the result from [LS2], where the kinetic energy is described by  $-\Delta/2$ , whereas it is  $-\Delta$  in our case.)

Let us fix  $N \in \mathbb{N}$ . Given  $\psi \in H^1(\mathbb{R}^{3N})$  with  $\int_{\mathbb{R}^{3N}} |\psi|^2 dx = 1$  we define  $\tilde{\psi}(x, y) = \psi(x)\psi(y)$  for  $x, y \in \mathbb{R}^{3N}$  and let  $e = (1, \dots, 1, -1, \dots, -1)$ , where both 1 and  $-1$  are repeated  $N$  times. Then, from (1.1),

$$\left( \tilde{\psi}, H^{(2N)}(e) \tilde{\psi} \right) = 2 \mathcal{E}_1^{(N)}[\psi] \quad \text{and} \quad \int_{\mathbb{R}^{6N}} |\tilde{\psi}|^2 dx dy = 1.$$

Thus, we conclude that

$$2E_1^{(b)}(N) = \inf_{\psi} 2 \mathcal{E}_1^{(N)}[\psi] \geq \inf_{e \in \{-1, 1\}^N} \inf \text{spec } H^{(2N)}(e).$$

The lower bound (1.3) in Theorem 1.1 thus follows from (2.1).

**2.2. The upper bound.**

**2.2.1. Introduction.** Most of this paper is taken up with the upper bound in Theorem 1.1. Normally, upper bounds are easier than lower bounds, but this is not necessarily so for Coulomb systems where we want not just an asymptotic power law but also an accurate constant multiplying the power law. The truly remarkable fact is that the accurate constants were first found by Foldy [Fo] for the one-component plasma (jellium) using Bogolubov's method, and for the two-component gas by Dyson [D] using Foldy's result. None of this was rigorous, however. The rigorous lower bounds were done in [LS1, LS2]. The upper bounds were done by Solovej in a tour de force [S]. Our work here consists largely in imitating and adapting Solovej's work to our special case.

As Solovej points out, Foldy's calculation, while not yielding a rigorous lower bound, essentially yields a rigorous upper bound – much as Pekar's model is a rigorous upper bound for Fröhlich's model (1.7). Unfortunately, this is not quite so simple since one of the things done in [Fo] is to use periodic boundary conditions (which is not easy to justify for Coulomb systems). Another hard to justify procedure is to mimic the charge

neutralizing background by simply discarding the  $k = 0$  term in the Fourier series for the Coulomb potential. It was Solovej who succeeded in solving these problems.

Bogolubov's method of 1947 [Bo] takes account of bosonic symmetry using boson creation and annihilation operators in momentum space. The Coulomb interaction is, like any 2-body interaction, represented by a quartic in these operators. Bogolubov's idea is to retain only those terms that have no more than two operators of non-zero momentum and to replace the zero momentum operators by  $\sqrt{N}$  (see [LSY]). The resulting quadratic in non-zero momentum operators is then diagonalized. This latter process can be thought of as using 'squeezed coherent states'.

**2.2.2. First Step.** In our proof of the upper bound, we shall linearize the non-linear functional  $\mathcal{E}_1^{(N)}[\cdot]$ , as in [FLST]. This process replaces the 2-body interaction by a one-body potential, so that the problem tends to resemble the one-component Coulomb gas. Given a real-valued function  $\sigma$  on  $\mathbb{R}^3$  with  $D(\sigma, \sigma) < \infty$  we introduce the operator

$$H_\sigma^{(N)} = \sum_{j=1}^N (-\Delta_j - \sigma * |x_j|^{-1}) + \sum_{i < j} |x_i - x_j|^{-1} + D(\sigma, \sigma) \quad \text{in } L_{\text{symm}}^2(\mathbb{R}^{3N}),$$

where  $\sigma * |x_j|^{-1}$  is an abbreviation for  $(\sigma * |\cdot|^{-1})(x_j)$ . Then by linearization we mean that

$$\inf_{\sigma} \inf \text{spec } H_\sigma^{(N)} = E_1^{(b)}(N), \quad (2.2)$$

as is easily verified by completing a square.

We denote by  $\mathcal{F}(L^2(\mathbb{R}^3))$  the bosonic Fock space over  $L^2(\mathbb{R}^3)$  and consider the operator

$$\mathcal{H}_\sigma = \bigoplus_{N=0}^{\infty} H_\sigma^{(N)} \quad \text{in } \mathcal{F}(L^2(\mathbb{R}^3))$$

(with  $H_\sigma^{(0)} = 0$  and  $H_\sigma^{(1)} = -\Delta - \sigma * |x|^{-1} + D(\sigma, \sigma)$ .) As usual, we denote by  $\mathcal{N}$  the number operator.

In order to prove the upper bound in Theorem 1.1, our strategy will be to find an upper bound on  $\inf_{\sigma} \inf \text{spec } \mathcal{H}_\sigma$  of the required form. Indeed, the main ingredient in the proof of Theorem 1.1 is the following proposition.

**Proposition 2.1.** *For any sufficiently large  $n$  there is a normalized  $\Psi_n \in \mathcal{F}(L^2(\mathbb{R}^3))$  with finite kinetic energy and a  $\sigma_n$  with  $D(\sigma_n, \sigma_n) < \infty$  such that*

$$(\Psi_n, \mathcal{H}_{\sigma_n} \Psi_n) \leq -An^{7/5} (1 - Cn^{-1/35}), \quad (2.3)$$

$$(\Psi_n, \mathcal{N} \Psi_n) - n \leq Cn^{3/5}, \quad (2.4)$$

$$(\Psi_n, \mathcal{N}^2 \Psi_n) - (\Psi_n, \mathcal{N} \Psi_n)^2 \leq Cn, \quad (2.5)$$

where  $A$  is the constant from (1.4) and  $C$  is some constant independent of  $n$ .

Actually, instead of (2.4) and (2.5) we shall show the stronger facts that

$$|(\Psi_n, \mathcal{N} \Psi_n) - n| \leq Cn^{3/5} \quad (2.6)$$

$$(\Psi_n, \mathcal{N}^2 \Psi_n) - (\Psi_n, \mathcal{N} \Psi_n)^2 \leq n + Cn^{3/5+4/15}. \quad (2.7)$$

2.2.3. *From Proposition 2.1 to Theorem 1.1.* Accepting Proposition 2.1 for the moment, we now explain how this trial state  $\Psi_n$  on  $\mathcal{F}$  leads to an upper bound for  $E_1^{(b)}(N)$ . The following argument is taken from [S] and reproduced here for the sake of completeness.

*Proof of Theorem 1.1 given Proposition 2.1.* As a preliminary to the proof, we shall show that for all  $M > 0$  and all sufficiently large  $n$ ,

$$\sum_{m > (\Psi_n, \mathcal{N} \Psi_n) + M} m^{7/5} \|\Psi_n^{(m)}\|^2 \leq CM^{-3/5} n^{17/10}. \quad (2.8)$$

Here  $\Psi_n^{(m)}$  denotes the projection of  $\Psi_n$  onto the sector of  $m$  particles.

Indeed, by Hölder's inequality,

$$\begin{aligned} \sum_{m > (\Psi_n, \mathcal{N} \Psi_n) + M} m^{7/5} \|\Psi_n^{(m)}\|^2 &\leq M^{-3/5} \sum_{m=0}^{\infty} m^{7/5} |m - (\Psi_n, \mathcal{N} \Psi_n)|^{3/5} \|\Psi_n^{(m)}\|^2 \\ &\leq M^{-3/5} (\Psi_n, \mathcal{N}^2 \Psi_n)^{7/10} ((\Psi_n, \mathcal{N}^2 \Psi_n) - (\Psi_n, \mathcal{N} \Psi_n)^2)^{3/10}. \end{aligned}$$

It follows from (2.4) and (2.5) that

$$(\Psi_n, \mathcal{N}^2 \Psi_n) \leq Cn^2 \quad \text{and} \quad (\Psi_n, \mathcal{N}^2 \Psi_n) - (\Psi_n, \mathcal{N} \Psi_n)^2 \leq Cn.$$

This proves (2.8).  $\square$

*We now return to the proof of Theorem 1.1.* Recalling the linearization formula (2.2) and using the fact that  $N \mapsto \inf \text{spec } H_\sigma^{(N)}$  is non-increasing and non-positive, we have for any  $n$ ,

$$\begin{aligned} E_1^{(b)}(N) &\leq \inf \text{spec } H_{\sigma_n}^{(N)} \leq (\inf \text{spec } H_{\sigma_n}^{(N)}) \sum_{m=0}^N \|\Psi_n^{(m)}\|^2 \leq \sum_{m=0}^N (\inf \text{spec } H_{\sigma_n}^{(m)}) \|\Psi_n^{(m)}\|^2 \\ &\leq \sum_{m=0}^N (\Psi_n^{(m)}, H_{\sigma_n}^{(m)} \Psi_n^{(m)}) = (\Psi_n, \mathcal{H}_{\sigma_n} \Psi_n) - \sum_{m=N+1}^{\infty} (\Psi_n^{(m)}, H_{\sigma_n}^{(m)} \Psi_n^{(m)}). \end{aligned}$$

Thus, we need a lower bound on the last sum. Because of the linearization formula (2.2) and the lower bound on  $E_1^{(b)}(m)$  proved above we have

$$\sum_{m=N+1}^{\infty} (\Psi_n^{(m)}, H_{\sigma_n}^{(m)} \Psi_n^{(m)}) \geq \sum_{m=N+1}^{\infty} \|\Psi_n^{(m)}\|^2 \mathcal{E}_1^{(m)}[\Psi_n^{(m)}] \geq -C \sum_{m=N+1}^{\infty} m^{7/5} \|\Psi_n^{(m)}\|^2.$$

For all  $N \in \mathbb{N}$  sufficiently large we shall apply the previous bounds with  $n = N - C_0 N^{3/5}$ . Here, by (2.4), the constant  $C_0$  can be chosen in such a way that for another constant  $C_1 > 0$  one has

$$(\Psi_n, \mathcal{N} \Psi_n) \leq N - C_1 N^{3/5}.$$

Then we can use (2.8) to bound

$$\begin{aligned}
-C \sum_{m=N+1}^{\infty} m^{7/5} \|\Psi_n^{(m)}\|^2 &\geq -C \sum_{m > (\Psi_n, \mathcal{N}\Psi_n) + C_1 N^{3/5}} m^{7/5} \|\Psi_n^{(m)}\|^2 \\
&\geq -CN^{-9/25} n^{17/10} \\
&\geq -CN^{7/5-3/50}.
\end{aligned}$$

Using (2.3) we conclude that

$$N^{-7/5} E_1^{(b)}(N) \leq -A (1 - C_0 N^{-2/5})^{7/5} (1 - CN^{-1/35}) + CN^{-3/50} \leq A (1 - CN^{-1/35}).$$

This proves (1.6) and completes the proof of Theorem 1.1.

**2.2.4. Proof of Proposition 2.1, Step 1.** Thus, we have reduced the proof of the upper bound in Theorem 1.1 to the proof of Proposition 2.1. The following lemma guarantees the existence of an appropriate trial state.

**Lemma 2.2.** *For any real  $\varphi \in H^1(\mathbb{R}^3)$  and any non-negative, real trace class operator  $\gamma$  with finite kinetic energy there is a normalized  $\Psi \in \mathcal{F}(L^2(\mathbb{R}^3))$  with finite kinetic energy and a  $\sigma$  with  $D(\sigma, \sigma) < \infty$  such that*

$$\begin{aligned}
(\Psi, \mathcal{H}_\sigma \Psi) &= (\varphi, -\Delta \varphi) + \text{Tr}(-\Delta) \gamma - \text{Tr} K_\varphi \left( \sqrt{\gamma(\gamma+1)} - \gamma \right) \\
&\quad + \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\gamma(x, x')|^2}{|x - x'|} dx dx' \\
&\quad + \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\sqrt{\gamma(\gamma+1)}(x, x')|^2}{|x - x'|} dx dx', \tag{2.9}
\end{aligned}$$

$$(\Psi, \mathcal{N}\Psi) = \|\varphi\|^2 + \text{Tr} \gamma, \tag{2.10}$$

$$(\Psi, \mathcal{N}^2 \Psi) - (\Psi, \mathcal{N}\Psi)^2 = \|\varphi\|^2 + 2 \text{Tr} \gamma(\gamma+1) - 2(\varphi, \sqrt{\gamma(\gamma+1)} \varphi) + 2(\varphi, \gamma \varphi). \tag{2.11}$$

Here,  $K_\varphi$  is the integral operator with integral kernel  $K_\varphi(x, x') = \varphi(x)|x - x'|^{-1}\varphi(x')$ .

*Proof.* We write  $\gamma = \sum_{\alpha=1}^{\infty} \frac{\lambda_\alpha^2}{1-\lambda_\alpha^2} |\psi_\alpha\rangle\langle\psi_\alpha|$  with  $0 < \lambda_\alpha < 1$  and  $(\psi_\alpha)$  orthonormal. Since  $\gamma$  is real, the  $\psi_\alpha$  can be chosen real. Following [S] we set

$$\Psi = \prod_{\alpha} \left( (1 - \lambda_\alpha^2)^{1/4} \exp \left( -\frac{\lambda_\alpha}{2} (a(\psi_\alpha)^* - (\varphi, \psi_\alpha)) (a(\psi_\alpha)^* - (\varphi, \psi_\alpha)) \right) \right) |\varphi\rangle_C$$

with

$$|\varphi\rangle_C = \exp \left( -\frac{1}{2} \|\varphi\|^2 + a(\varphi)^* \right) |0\rangle.$$

Here  $a$  and  $a^*$  are (bosonic) annihilation and creation operators on  $\mathcal{F}(L^2(\mathbb{R}^3))$ . One can check that  $\|\Psi\| = 1$ . Equations (2.10) and (2.11) follow from [S, (23), (24)]. (Note

that the last two terms on the right side of (2.11) are absent in [S], since there  $\gamma\varphi = 0$ . Moreover, as in [S, (58), (59) and (60)], we find

$$\begin{aligned} \left( \Psi, \bigoplus_{N=0}^{\infty} \sum_{j=1}^N (-\Delta_j - \sigma * |x_j|^{-1}) \Psi \right) &= \|\nabla\varphi\|^2 + \text{Tr}(-\Delta - \sigma * |x|^{-1})\gamma \\ &= \|\nabla\varphi\|^2 + \text{Tr}(-\Delta)\gamma - 2D(\sigma, \rho_\gamma) \end{aligned}$$

and that

$$\begin{aligned} \left( \Psi, \bigoplus_{N=0}^{\infty} \sum_{i < j} |x_i - x_j|^{-1} \Psi \right) &= -\text{Tr} K_\varphi \left( \sqrt{\gamma(\gamma+1)} - \gamma \right) \\ &\quad + D(\varphi^2, \varphi^2) + 2D(\rho_\gamma, \varphi^2) + D(\rho_\gamma, \rho_\gamma) \\ &\quad + \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\gamma(x, x')|^2}{|x - x'|} dx dx' + \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\sqrt{\gamma(\gamma+1)}(x, x')|^2}{|x - x'|} dx dx'. \end{aligned}$$

With the choice  $\sigma = \varphi^2 + \rho_\gamma$  we obtain (2.9).  $\square$

**2.2.5. Proof of Proposition 2.1, Step 2.** This reduces our task of proving Proposition 2.1 to finding corresponding  $\varphi$  and  $\gamma$ . We will do this using the method of coherent states; see, e.g., [LL, Sec. 12]. Given a real, even function  $G \in H^1(\mathbb{R}^3)$  with  $\|G\| = 1$  we let

$$G_{p,q}(x) = e^{ip \cdot x} G(x - q), \quad p, q, x \in \mathbb{R}^3.$$

Let  $M$  be a non-negative, integrable function on  $\mathbb{R}^3 \times \mathbb{R}^3$  satisfying  $M(p, q) = M(-p, q)$  and define the operator

$$\gamma = \iint_{\mathbb{R}^3 \times \mathbb{R}^3} M(p, q) |G_{p,q}\rangle \langle G_{p,q}| \frac{dp dq}{(2\pi)^3}.$$

Clearly,  $\gamma$  is a real, non-negative trace class operator. Let  $\varphi \in H^1(\mathbb{R}^3)$  be real. Then Lemma 2.2 yields a trial state  $\Psi$  and a  $\sigma$  with

$$(\Psi, \mathcal{H}_\sigma \Psi) = (\varphi, -\Delta\varphi) + \text{Tr}(-\Delta)\gamma - \text{Tr} K_\varphi \left( \sqrt{\gamma(\gamma+1)} - \gamma \right) + \mathcal{R}_{\text{xc}},$$

where

$$\mathcal{R}_{\text{xc}} = \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\gamma(x, x')|^2}{|x - x'|} dx dx' + \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\sqrt{\gamma(\gamma+1)}(x, x')|^2}{|x - x'|} dx dx'.$$

By [LL, Thm. 12.9]

$$\text{Tr}(-\Delta)\gamma = \text{Tr}(-\Delta - \|\nabla G\|^2)\gamma + \mathcal{R}_{\text{loc}} = \iint_{\mathbb{R}^3 \times \mathbb{R}^3} p^2 M(p, q) \frac{dp dq}{(2\pi)^3} + \mathcal{R}_{\text{loc}},$$

where

$$\mathcal{R}_{\text{loc}} = \|\nabla G\|^2 \text{Tr} \gamma = \|\nabla G\|^2 \iint_{\mathbb{R}^3 \times \mathbb{R}^3} M(p, q) \frac{dp dq}{(2\pi)^3}.$$



Moreover, since  $t \mapsto \sqrt{t(t+1)} - t$  is operator-concave, Solovej's operator version of the Berezin–Lieb inequality [S, Thm. A.1] yields

$$\begin{aligned} \text{Tr } K_\varphi \left( \sqrt{\gamma(\gamma+1)} - \gamma \right) \\ \geq \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \left( \sqrt{M(p,q)(M(p,q)+1)} - M(p,q) \right) (G_{p,q}, K_\varphi G_{p,q}) \frac{dp dq}{(2\pi)^3}. \end{aligned}$$

It is not unreasonable to think that  $(G_{p,q}, K_\varphi G_{p,q})$  should be an approximation to  $4\pi\varphi(q)^2|p|^{-2}$ , and therefore we introduce the remainder

$$\mathcal{R}_{\text{int}} = \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \left( \sqrt{M(p,q)(M(p,q)+1)} - M(p,q) \right) \left( \frac{4\pi\varphi(q)^2}{|p|^2} - (G_{p,q}, K_\varphi G_{p,q}) \right) \frac{dp dq}{(2\pi)^3}.$$

Thus, we have

$$(\Psi, \mathcal{H}_\sigma \Psi) = \mathcal{E}(\varphi, M) + \mathcal{R}_{\text{loc}} + \mathcal{R}_{\text{int}} + \mathcal{R}_{\text{xc}}$$

where

$$\begin{aligned} \mathcal{E}(\varphi, M) = & \|\nabla \varphi\|^2 + \iint_{\mathbb{R}^3 \times \mathbb{R}^3} p^2 M(p,q) \frac{dp dq}{(2\pi)^3} \\ & - 4\pi \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \left( \sqrt{M(p,q)(M(p,q)+1)} - M(p,q) \right) \frac{\varphi(q)^2}{p^2} \frac{dp dq}{(2\pi)^3}. \end{aligned}$$

*Minimizing  $\mathcal{E}(\varphi, M)$ .* In order to make our upper bound as small as possible, we would like to minimize the functional  $\mathcal{E}(\varphi, M)$  with respect to functions  $M \geq 0$  and  $\varphi \in H^1(\mathbb{R}^3)$  satisfying the requirements above. Carrying out the minimization over  $M$  yields

$$M_*(p, q) = g \left( \frac{|p|}{(4\pi)^{1/4} \varphi(q)^{1/2}} \right), \quad \text{where} \quad g(a) = \frac{1}{2} \left( \frac{a^4 + 1}{\sqrt{a^4(a^4 + 2)}} - 1 \right). \quad (2.12)$$

With this choice of  $M$  we obtain

$$\begin{aligned} & \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \left( p^2 M_*(p, q) - \frac{4\pi\varphi(q)^2}{p^2} \left( \sqrt{M_*(p, q)(M_*(p, q)+1)} - M_*(p, q) \right) \right) \frac{dp dq}{(2\pi)^3} \\ &= \left( \frac{4}{\pi} \right)^{3/4} \int_{\mathbb{R}^3} |\varphi(q)|^{5/2} dq \int_0^\infty \left( a^4 g - \left( \sqrt{g(g+1)} - g \right) \right) da \\ &= -2^{1/2} \pi^{-3/4} \int_{\mathbb{R}^3} |\varphi(q)|^{5/2} dq \int_0^\infty \left( a^4 + 1 - a^2 \sqrt{a^4 + 2} \right) da \\ &= -\frac{2}{5} \left( \frac{2}{\pi} \right)^{1/4} \frac{\Gamma(3/4)}{\Gamma(5/4)} \int_{\mathbb{R}^3} |\varphi(q)|^{5/2} dq \\ &= -I_0 \int_{\mathbb{R}^3} |\varphi(q)|^{5/2} dq, \end{aligned}$$

with  $I_0$  from (1.5). Thus,

$$\mathcal{E}(\varphi, M_*) = \|\nabla \varphi\|^2 - I_0 \int_{\mathbb{R}^3} |\varphi(q)|^{5/2} dq. \quad (2.13)$$

The latter functional has a minimizer for any fixed value of  $\|\varphi\|^2$  and the minimizer is non-negative. (This is a well-known result in the calculus of variations – in fact, for us the existence of a minimizer is not really necessary and we could simply work with almost-minimizers.) Thus, let us introduce a parameter  $n > 0$  and let us choose  $\varphi_*$  to be the minimizer of (2.13) under the constraint  $\|\varphi\|^2 = n$ . Then, by scaling,

$$\varphi_*(x) = n^{4/5} \Phi(n^{1/5}x)$$

for a universal function  $\Phi$  with  $\|\Phi\| = 1$ , and (2.13) is equal to  $-An^{7/5}$  with  $A$  from (1.4).

Moreover, if  $M_*$  is chosen according to (2.12), then

$$\mathrm{Tr} \gamma = \iint_{\mathbb{R}^3 \times \mathbb{R}^3} M_*(p, q) \frac{dp dq}{(2\pi)^3} = \frac{(4\pi)^{3/4}}{2\pi^2} \int_{\mathbb{R}^3} \varphi_*(q)^{3/2} dq \int_0^\infty g(a) a^2 da = Cn^{3/5}.$$

(The fact that  $\Phi \in L^{3/2}$  follows from the fact that  $\Phi$  is exponentially decaying, as can be verified using the Euler–Lagrange equation satisfied by  $\Phi$ .) Thus, from (2.9) we obtain

$$(\Psi, \mathcal{N}\Psi) = n + Cn^{3/5}.$$

*Definition of  $\gamma_{n,\varepsilon}$ .* The problem with the above argument is that we cannot get a good bound on  $\mathrm{Tr} \gamma^2$ , which is needed in order to control the fluctuations of the particle number of  $\Psi$ , see (2.11). Therefore, we shall introduce  $g_\varepsilon(a) = 0$  if  $a \leq \varepsilon$  and  $g_\varepsilon(a) = g(a)$  if  $a > \varepsilon$ . We denote by  $\Psi_{n,\varepsilon}$  the state constructed in Lemma 2.2 corresponding to  $\gamma_{n,\varepsilon}$  which is given in terms of

$$M_{n,\varepsilon}(p, q) = g_\varepsilon \left( \frac{|p|}{(4\pi)^{1/4} n^{2/5} \Phi(n^{1/5}q)^{1/2}} \right).$$

Then, as before,  $\gamma_{n,\varepsilon}$  is trace class with

$$\mathrm{Tr} \gamma_{n,\varepsilon} = \frac{(4\pi)^{5/4}}{2\pi^2} \int_{\mathbb{R}^3} \varphi(q)^{3/2} dq \int_\varepsilon^\infty g(a) a^2 da \leq Cn^{3/5}, \quad (2.14)$$

with  $C$  independent of  $\varepsilon$ . In view of (2.10) this implies (2.6), which in turn implies (2.4).

The advantage of introducing the parameter  $\varepsilon > 0$  is that now, by the Berezin–Lieb inequality [B, L],

$$\mathrm{Tr} \gamma_{n,\varepsilon}^2 \leq \iint_{\mathbb{R}^3 \times \mathbb{R}^3} M(p, q)^2 \frac{dp dq}{(2\pi)^3} = \frac{(4\pi)^{3/4}}{2\pi^2} \int_{\mathbb{R}^3} \varphi(q)^{3/2} dq \int_\varepsilon^\infty g(a)^2 a^2 da \leq C\varepsilon^{-1} n^{3/5}. \quad (2.15)$$

(In the final inequality we used the fact that  $g(a)$  diverges like  $a^{-2}$  as  $a \rightarrow 0$ .) Thus,

$$0 \leq 2 \mathrm{Tr} \gamma_{n,\varepsilon} (\gamma_{n,\varepsilon} + 1) \leq C\varepsilon^{-1} n^{3/5}.$$

We will later choose  $\varepsilon = n^{-4/15}$ . Then, in view of (2.11), and since  $(\varphi, \sqrt{\gamma(\gamma+1)}\varphi) \geq (\varphi, \gamma\varphi)$ , this implies (2.7), which in turn implies (2.5).

Thus, to complete the proof of Proposition 2.1, we need to verify that, if  $\varepsilon$  is chosen suitably as function of  $n$ , then

$$(\Psi_{n,\varepsilon}, \mathcal{H}\Psi_{n,\varepsilon}) \leq -An^{7/5}(1 - Cn^{-1/35}) \quad \text{as } n \rightarrow \infty. \quad (2.16)$$

Note that by repeating the previous argument we find that

$$\begin{aligned} \mathcal{E}(\varphi, M_{n,\varepsilon}) &= \|\nabla\varphi\|^2 - I_\varepsilon\|\varphi\|_{5/2}^{5/2} \\ &= \left(\|\nabla\varphi\|^2 - I_0\|\varphi\|_{5/2}^{5/2}\right) + (I_0 - I_\varepsilon)\|\varphi\|_{5/2}^{5/2} \\ &= -An^{7/5} + \mathcal{R}_{\text{main}}, \end{aligned}$$

where

$$\begin{aligned} -I_\varepsilon &= \left(\frac{4}{\pi}\right)^{3/4} \int_\varepsilon^\infty \left(a^4 g - \left(\sqrt{g(g+1)} - g\right)\right) da \\ &= -2^{1/2}\pi^{-3/4} \int_{\mathbb{R}^3} |\varphi(q)|^{5/2} dq \int_\varepsilon^\infty \left(a^4 + 1 - a^2\sqrt{a^4+2}\right) da \end{aligned}$$

and

$$\mathcal{R}_{\text{main}} = (I_0 - I_\varepsilon)\|\varphi\|_{5/2}^{5/2}.$$

This will prove (2.16), provided we can show that, for an appropriate choice of the function  $G$ , the errors  $\mathcal{R}_{\text{main}}$ ,  $\mathcal{R}_{\text{loc}}$ ,  $\mathcal{R}_{\text{int}}$  and  $\mathcal{R}_{\text{xc}}$  are at most  $O(n^{7/5-1/35})$ . To do so, we choose  $G(x) = (\pi\ell)^{-3/2} \exp(-(x/\ell)^2)$  with a parameter  $\ell > 0$  to be determined.

*Bound on  $\mathcal{R}_{\text{main}}$ .* Since  $a^4 + 1 + a^2\sqrt{a^4+2}$  is finite near  $a = 0$  and since, by scaling,  $\|\varphi\|_{5/2}^{5/2} = n^{7/5}\|\Phi\|_{5/2}^{5/2}$ , we have

$$\mathcal{R}_{\text{main}} \leq C\varepsilon n^{7/5}.$$

*Bound on  $\mathcal{R}_{\text{loc}}$ .* Clearly, by (2.14) we have

$$\mathcal{R}_{\text{loc}} = \|\nabla G\|^2 \iint_{\mathbb{R}^3 \times \mathbb{R}^3} M_{n,\varepsilon}(p, q) \frac{dp dq}{(2\pi)^3} \leq C\ell^{-2}n^{3/5} = Cn^{7/5}(n^{2/5}\ell)^{-2}.$$

*Bound on  $\mathcal{R}_{\text{int}}$ .* This bound can be taken literally from [S, (47)],

$$\mathcal{R}_{\text{int}} \leq Cn^{7/5} \left( (n^{2/5}\ell)^{-1/2} + (n^{2/5}\ell)^3 n^{-1/5} \right).$$

(The constant here can be chosen independently of  $\varepsilon \in (0, 1]$ .)

*Bound on  $\mathcal{R}_{\text{xc}}$ .* Here we argue as in Solovej's analysis of the one-component gas; see [S, (67)]. Hardy's inequality yields

$$\begin{aligned} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\gamma_{n,\varepsilon}(x, x')|^2}{|x - x'|} dx dx' &\leq \left( \iint_{\mathbb{R}^3 \times \mathbb{R}^3} |\gamma_{n,\varepsilon}(x, x')|^2 dx dx' \right)^{1/2} \\ &\quad \times \left( \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\gamma_{n,\varepsilon}(x, x')|^2}{|x - x'|^2} dx dx' \right)^{1/2} \\ &\leq 2 (\text{Tr } \gamma_{n,\varepsilon}^2)^{1/2} (\text{Tr } (-\Delta) \gamma_{n,\varepsilon}^2)^{1/2}. \end{aligned}$$

According to (2.15) we have  $\text{Tr} \gamma_{n,\varepsilon}^2 \leq C\varepsilon^{-1}n^{3/5}$ . Moreover, by Solovej's operator-version of the Berezin–Lieb inequality [S, Thm. A.1], we have

$$\begin{aligned} \text{Tr}(-\Delta)\gamma_{n,\varepsilon}^2 &\leq \iint_{\mathbb{R}^3 \times \mathbb{R}^3} M_{n,\varepsilon}(p, q)^2 (G_{p,q}, (-\Delta)G_{p,q}) \frac{dp dq}{(2\pi)^3} \\ &= \iint_{\mathbb{R}^3 \times \mathbb{R}^3} M_{n,\varepsilon}(p, q)^2 (p^2 + \|\nabla G\|^2) \frac{dp dq}{(2\pi)^3} \\ &\leq C (n^{7/5} + \varepsilon^{-1}\ell^{-2}n^{3/5}) . \end{aligned}$$

(Here we used the fact that  $\int_0^\infty a^4 g(a)^2 da < \infty$  to bound the term involving  $p^2$ , as well as (2.15) to bound the term involving  $\|\nabla G\|^2$ .) Thus,

$$\iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\gamma_{n,\varepsilon}(x, x')|^2}{|x - x'|} dx dx' \leq C\varepsilon^{-1/2}n^{7/5-2/5} \left(1 + \varepsilon^{-1/2} (n^{2/5}\ell)^{-1}\right) .$$

The term that involves  $\sqrt{\gamma_{n,\varepsilon}(\gamma_{n,\varepsilon} + 1)}$  instead of  $\gamma_{n,\varepsilon}$  can be bounded similarly and we finally obtain

$$\mathcal{R}_{\text{xc}} \leq C\varepsilon^{-1/2}n^{7/5-2/5} \left(1 + \varepsilon^{-1/2} (n^{2/5}\ell)^{-1}\right) .$$

In order to minimize the remainder in  $\mathcal{R}_{\text{int}}$  we choose  $\ell = n^{-2/5+2/35}$  and find  $\mathcal{R}_{\text{int}} \leq Cn^{7/5-1/35}$  and  $\mathcal{R}_{\text{loc}} \leq Cn^{7/5-4/35}$ . In order to minimize the error coming from  $\mathcal{R}_{\text{main}}$  and  $\mathcal{R}_{\text{xc}}$  we choose  $\varepsilon = n^{-4/15}$  and find  $\mathcal{R}_{\text{main}} \leq Cn^{7/5-4/15}$  and  $\mathcal{R}_{\text{xc}} \leq Cn^{7/5-4/15}$ . As explained above, this proves (2.16) and finishes the proof of Theorem 1.1.  $\square$

## APPENDIX A. PROOF OF THEOREM 1.3

Since [GM] have already shown the upper bound, we only need to show the lower bound. In fact, we shall show the lower bound

$$\mathcal{E}_{U,\alpha}^{(N)}[\psi] \geq N^{7/3}e_U^{(f)} - C(1-U)^2N^{7/3-2/33} \left(1 + N^{-40/33}(U/(1-U))^2\right) . \quad (\text{A.1})$$

Using the Lieb–Oxford inequality [LO] we bound from below

$$\mathcal{E}_U^{(N)}[\psi] \geq \text{Tr}(-\Delta)\gamma_\psi - (1-U)D(\rho_\gamma, \rho_\gamma) - 1.68 U \int_{\mathbb{R}^3} \rho_\gamma^{4/3} dx ,$$

where

$$\gamma_\psi(x, x') = \int \cdots \int_{\mathbb{R}^{3(N-1)}} \overline{\psi(x, x_2, \dots, x_N)} \psi(x', x_2, \dots, x_N) dx_2 \dots dx_N$$

denotes the one-particle density matrix. Thus, for any  $G \in H^1(\mathbb{R}^3)$  and any  $0 < \varepsilon < 1$ ,

$$\mathcal{E}_U^{(N)} \geq (1-\varepsilon) \text{Tr}(-\Delta + \|\nabla G\|^2)\gamma_\psi - (1-U)D(\rho_\psi * |G|^2, \rho_\psi * |G|^2) + \varepsilon \mathcal{T} - \mathcal{R}_{\text{loc}} - \mathcal{R}_{\text{rep}} - \mathcal{R}_{\text{xc}} ,$$

where

$$\begin{aligned}\mathcal{T} &= \text{Tr}(-\Delta)\gamma_\psi, \\ \mathcal{R}_{\text{loc}}^{(\varepsilon)} &= (1 - \varepsilon)\|\nabla G\|^2 \text{Tr} \gamma_\psi = (1 - \varepsilon)N\|\nabla G\|^2, \\ \mathcal{R}_{\text{rep}} &= -(1 - U) \left( D(\rho_\psi * |G|^2, \rho_\psi * |G|^2) - D(\rho_\psi, \rho_\psi) \right), \\ \mathcal{R}_{\text{xc}}^{(\varepsilon)} &= 1.68 U \int_{\mathbb{R}^3} \rho_\gamma^{4/3} dx.\end{aligned}$$

Now assume again the  $G$  is real, even and normalized and let  $G_{p,q}$  be the corresponding coherent states. Set

$$M(p, q) = (G_{p,q}, \gamma_\psi G_{p,q}).$$

Then  $0 \leq \gamma_\psi \leq 1$  implies that  $0 \leq M \leq 1$ . We now observe that for any number  $\rho > 0$ ,

$$\inf \left\{ \int_{\mathbb{R}^3} p^2 m(p) \frac{dp}{(2\pi)^3} : 0 \leq m \leq 1, \int_{\mathbb{R}^3} m(p) \frac{dp}{(2\pi)^3} = \rho \right\} = \frac{3}{5} (6\pi^2)^{2/3} \rho^{5/3}.$$

(In fact, the infimum is attained iff  $m(p) = \chi_{\{p^2 < (6\pi^2 \rho)^{2/3}\}}$ .) Since  $\int_{\mathbb{R}^3} M(p, q) \frac{dp}{(2\pi)^3} = (\rho_\psi * G^2)(q)$  for any  $q \in \mathbb{R}^3$ , we obtain the lower bound

$$\text{Tr}(-\Delta + \|\nabla g\|^2)\gamma_\psi = \iint_{\mathbb{R}^3 \times \mathbb{R}^3} p^2 M(p, q) \frac{dp dq}{(2\pi)^3} \geq \frac{3}{5} (6\pi^2)^{2/3} \int_{\mathbb{R}^3} (\rho_\gamma * G^2)^{5/3} dx.$$

Thus,

$$\begin{aligned}\mathcal{E}_U^{(N)}[\psi] &\geq (1 - \varepsilon) \frac{3}{5} (6\pi^2)^{2/3} \int_{\mathbb{R}^3} (\rho_\gamma * G^2)^{5/3} dx - (1 - U) D(\rho_\gamma * G^2, \rho_\gamma * G^2) \\ &\quad + \varepsilon \mathcal{T} - \mathcal{R}_{\text{loc}} - \mathcal{R}_{\text{rep}} - \mathcal{R}_{\text{xc}} \\ &\geq (1 - \varepsilon)^{-1} N^{7/3} e_U^{(f)} + \varepsilon \mathcal{T} - \mathcal{R}_{\text{loc}} - \mathcal{R}_{\text{rep}} - \mathcal{R}_{\text{xc}} \\ &\geq N^{7/3} e_U^{(f)} + \varepsilon \mathcal{T} - \mathcal{R}_{\text{main}} - \mathcal{R}_{\text{loc}} - \mathcal{R}_{\text{rep}} - \mathcal{R}_{\text{xc}}.\end{aligned}$$

with

$$\mathcal{R}_{\text{main}} = \frac{\varepsilon}{1 - \varepsilon} N^{7/3} |e_U^{(f)}|.$$

In the second inequality above we used scaling to conclude that

$$\begin{aligned}\inf \left\{ (1 - \varepsilon) \frac{3}{5} (6\pi^2)^{2/3} \int_{\mathbb{R}^3} \sigma^{5/3} dx - (1 - U) D(\sigma, \sigma) : \sigma \geq 0, \int_{\mathbb{R}^3} \sigma dx = N \right\} \\ = (1 - \varepsilon)^{-1} N^{7/3} e_U^{(f)}.\end{aligned}$$

Thus, to obtain the claimed lower bound (A.1), it remains to show that  $G$  and  $\varepsilon$  can be chosen such that

$$\varepsilon \mathcal{T} - \mathcal{R}_{\text{main}} - \mathcal{R}_{\text{loc}} - \mathcal{R}_{\text{rep}} - \mathcal{R}_{\text{xc}} \geq -C(1 - U)^2 N^{7/3-2/33} (1 + N^{-40/33} (U/(1 - U))^2)$$

We bound the positive term  $\mathcal{T}$  from below by the Lieb–Thirring inequality [LT],

$$\mathcal{T} \geq K \int_{\mathbb{R}^3} \rho_\psi^{5/3} dx,$$

for some positive constant  $K$ . Since, by scaling,  $e_U^{(f)}$  is proportional to  $-N^{7/3}(1-U)^2$ , we have

$$\mathcal{R}_{\text{main}} \leq C\varepsilon N^{7/3}(1-U)^2.$$

To bound  $\mathcal{R}_{\text{loc}}$  and  $\mathcal{R}_{\text{rep}}$  we choose  $G(x) = \ell^{-3/2}g(x/\ell)$  with some  $\ell > 0$  to be determined and find that

$$\mathcal{R}_{\text{loc}} = (1-\varepsilon)N\ell^{-2}\|\nabla g\|^2 \leq N\ell^{-2}\|\nabla g\|^2.$$

Moreover, by Lemma A.1, if  $g$  is radial and has support in the unit ball, then

$$\mathcal{R}_{\text{int}} \leq C(1-U)\ell^{1/5}\|\rho_\psi\|_1\|\rho_\psi\|_{5/3} = C(1-U)\ell^{1/5}N\|\rho_\psi\|_{5/3}.$$

Finally, by Hölder,

$$\mathcal{R}_{\text{xc}} \leq 1.68 U\|\rho_\psi\|_1^{1/2}\|\rho_\psi\|_{5/3}^{5/6} = 1.68 UN^{1/2}\|\rho_\psi\|_{5/3}^{5/6}.$$

In order to balance the errors coming from the localization and the repulsion, we choose  $\ell$  proportional to  $((1-U)\|\rho_\psi\|_{5/3})^{-5/11}$ . To summarize, we have

$$\begin{aligned} \varepsilon\mathcal{T} - \mathcal{R}_{\text{main}} - \mathcal{R}_{\text{loc}} - \mathcal{R}_{\text{rep}} - \mathcal{R}_{\text{xc}} \\ \geq \varepsilon K\|\rho_\psi\|_{5/3}^{5/3} - C\left(\varepsilon(1-U)^2N^{7/3} + (1-U)^{10/11}N\|\rho_\psi\|_{5/3}^{10/11} + UN^{1/2}\|\rho_\psi\|_{5/3}^{5/6}\right). \end{aligned}$$

Minimizing  $(\varepsilon K/2)\|\rho_\psi\|_{5/3}^{5/3} - C(1-U)^{10/11}N\|\rho_\psi\|_{5/3}^{10/11}$  and  $(\varepsilon K/2)\|\rho_\psi\|_{5/3}^{5/3} - CUN^{1/2}\|\rho_\psi\|_{5/3}^{5/6}$  with respect to  $\|\rho_\psi\|_{5/3}$ , we obtain

$$\begin{aligned} \varepsilon\mathcal{T} - \mathcal{R}_{\text{main}} - \mathcal{R}_{\text{loc}} - \mathcal{R}_{\text{rep}} - \mathcal{R}_{\text{xc}} \\ \geq -C\left(\varepsilon(1-U)^2N^{7/3} + \varepsilon^{-6/5}(1-U)^2N^{11/5} + \varepsilon^{-1}U^2N\right). \end{aligned}$$

Finally, we the choice  $\varepsilon = N^{-2/33}$  we obtain (A.1). This proves the claimed lower bound, except for the following lemma that was used in the proof.

**Lemma A.1.** *Let  $\sigma$  be a non-negative, radially symmetric function with support in a ball of radius  $R > 0$  and  $\int_{\mathbb{R}^3} \sigma dx = 1$ . Then, for all  $\rho \in L^1(\mathbb{R}^3) \cap L^{5/3}(\mathbb{R}^3)$ ,*

$$0 \leq D(\rho, \rho) - D(\rho * \sigma, \rho * \sigma) \leq CR^{1/10}\|\rho\|_1\|\rho\|_{5/3}$$

*Proof.* The left inequality is easily verified in Fourier space, or by using Newton's theorem, and we concentrate on proving the right one. In fact, we shall show that

$$D(\rho - \rho * \sigma, \tau) \leq CR^{1/5}\|\rho\|_1\|\tau\|_{5/3}.$$

Then, writing

$$D(\rho, \rho) - D(\rho * \sigma, \rho * \sigma) = D(\rho - \rho * \sigma, \rho + \rho * \sigma)$$

and noting that  $\|\rho + \rho * \sigma\|_{5/3} \leq \|\rho\|_{5/3} + \|\rho * \sigma\|_{5/3} \leq 2\|\rho\|_{5/3}$ , we will obtain the inequality of the lemma.

Thus, it remains to prove the above inequality. By Hölder's and Young's inequality,

$$2D(\rho - \rho * \sigma, \tau) \leq \| |x|^{-1} * \rho * \sigma - |x|^{-1} * \rho \|_{5/2} \|\tau\|_{5/3} \leq \|\rho\|_1 \| |x|^{-1} * \sigma - |x|^{-1} \|_{5/2} \|\tau\|_{5/3}.$$

By Newton's theorem, we have  $0 \leq |x|^{-1} - |x|^{-1} * \sigma \leq |x|^{-1} \chi_{\{|x| < R\}}$ . Thus,

$$\| |x|^{-1} * \sigma - |x|^{-1} \|_{5/2}^{5/2} \leq \int_{\{|x| < R\}} \frac{dx}{|x|^{5/2}} = 8\pi R^{1/2}.$$

This proves the claimed inequality.  $\square$

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